Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:57 PM EDT

PDB ID	:	1D5B
Title	:	UNLIGANDED MATURE OXY-COPE CATALYTIC ANTIBODY
Authors	:	Mundorff, E.C.; Hanson, M.A.; Schultz, P.G.; Stevens, R.C.
Deposited on	:	1999-10-06
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

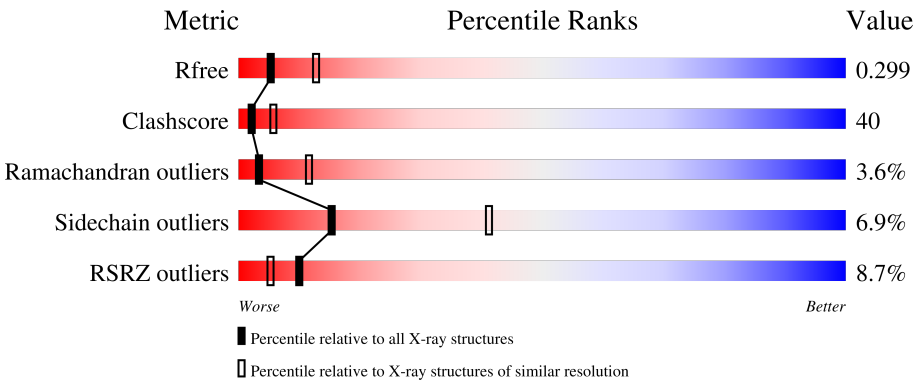
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	7% 36% 56% 7%
1	L	211	6% 40% 52% 8%
2	B	221	11% 51% 43% 5%
2	H	221	11% 48% 45% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6717 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called chimeric OXY-COPE catalytic ANTIBODY AZ-28 (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	1656	1040	273	336	7	0	0	0
1	L	211	1656	1040	273	336	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ASN	SER	conflict	UNP Q7TS98
A	51	THR	ALA	conflict	UNP Q7TS98
A	96	TYR	ARG	conflict	UNP Q7TS98
A	100	SER	GLY	conflict	UNP Q7TS98
L	34	ASN	SER	conflict	UNP Q7TS98
L	51	THR	ALA	conflict	UNP Q7TS98
L	96	TYR	ARG	conflict	UNP Q7TS98
L	100	SER	GLY	conflict	UNP Q7TS98

- Molecule 2 is a protein called chimeric OXY-COPE catalytic ANTIBODY AZ-28 (HEAVY chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	221	1665	1056	273	330	6	0	0	0
2	H	221	1665	1056	273	330	6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLN	-	expression tag	UNP K7T9I5
B	2	VAL	-	expression tag	UNP K7T9I5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLN	-	expression tag	UNP K7T9I5
B	4	LEU	-	expression tag	UNP K7T9I5
B	5	GLN	-	expression tag	UNP K7T9I5
B	6	GLN	-	expression tag	UNP K7T9I5
B	7	SER	-	expression tag	UNP K7T9I5
B	8	GLY	-	expression tag	UNP K7T9I5
B	32	PHE	TYR	conflict	UNP K7T9I5
B	56	GLY	SER	conflict	UNP K7T9I5
B	58	HIS	ASN	conflict	UNP K7T9I5
B	73	LYS	THR	conflict	UNP K7T9I5
B	95	GLY	GLU	conflict	UNP K7T9I5
B	96	HIS	VAL	conflict	UNP K7T9I5
B	97	SER	ARG	conflict	UNP K7T9I5
B	98	TYR	ARG	conflict	UNP K7T9I5
B	99	TYR	ARG	conflict	UNP K7T9I5
B	100	PHE	TYR	conflict	UNP K7T9I5
B	100B	ASP	ALA	conflict	UNP K7T9I5
B	100C	GLY	MET	conflict	UNP K7T9I5
H	1	GLN	-	expression tag	UNP K7T9I5
H	2	VAL	-	expression tag	UNP K7T9I5
H	3	GLN	-	expression tag	UNP K7T9I5
H	4	LEU	-	expression tag	UNP K7T9I5
H	5	GLN	-	expression tag	UNP K7T9I5
H	6	GLN	-	expression tag	UNP K7T9I5
H	7	SER	-	expression tag	UNP K7T9I5
H	8	GLY	-	expression tag	UNP K7T9I5
H	32	PHE	TYR	conflict	UNP K7T9I5
H	56	GLY	SER	conflict	UNP K7T9I5
H	58	HIS	ASN	conflict	UNP K7T9I5
H	73	LYS	THR	conflict	UNP K7T9I5
H	95	GLY	GLU	conflict	UNP K7T9I5
H	96	HIS	VAL	conflict	UNP K7T9I5
H	97	SER	ARG	conflict	UNP K7T9I5
H	98	TYR	ARG	conflict	UNP K7T9I5
H	99	TYR	ARG	conflict	UNP K7T9I5
H	100	PHE	TYR	conflict	UNP K7T9I5
H	100B	ASP	ALA	conflict	UNP K7T9I5
H	100C	GLY	MET	conflict	UNP K7T9I5

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	1	1	1	0	0

- Molecule 4 is water.

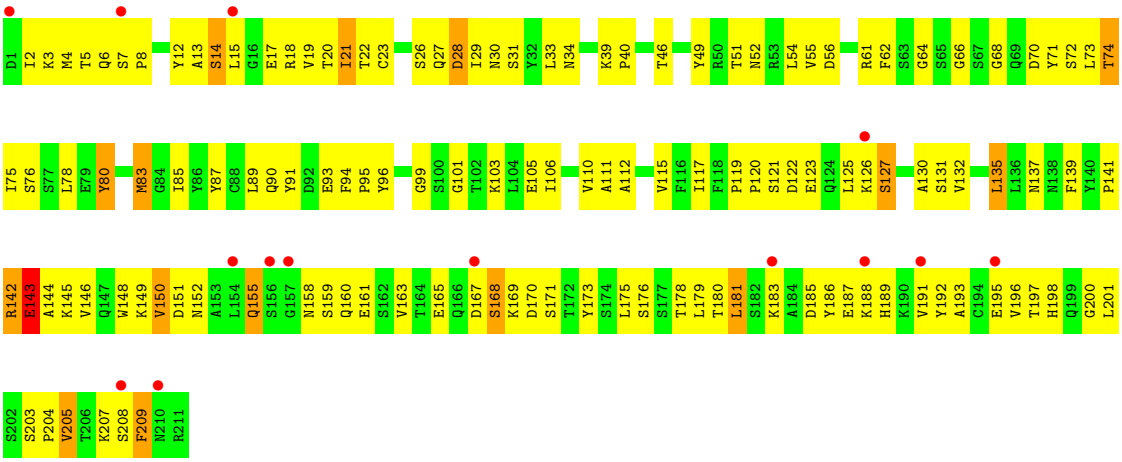
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	26	26	26	0	0
			Total	O		
4	B	13	13	13	0	0
			Total	O		
4	L	18	18	18	0	0
			Total	O		
4	H	17	17	17	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

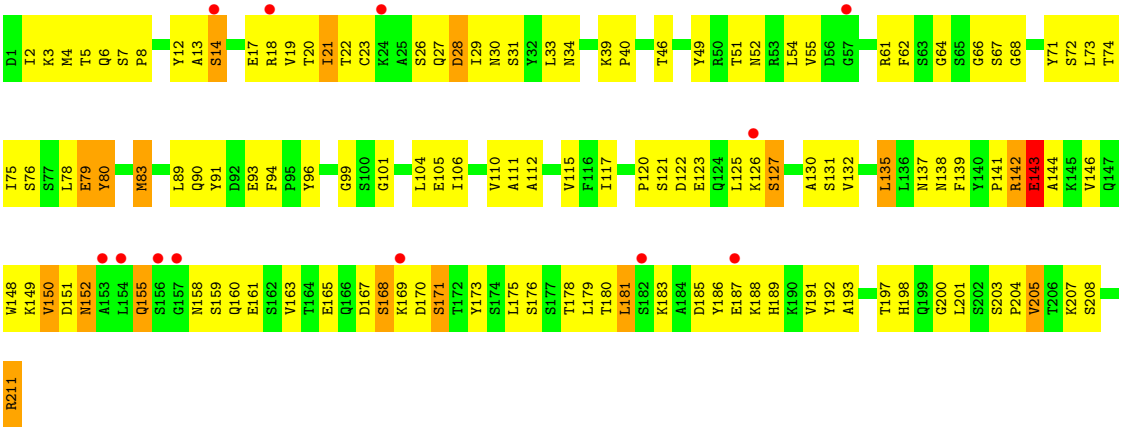
• Molecule 1: chimeric OXY-COPE catalytic ANTIBODY AZ-28 (light chain)

Chain A: 7% 36% 56% 7%



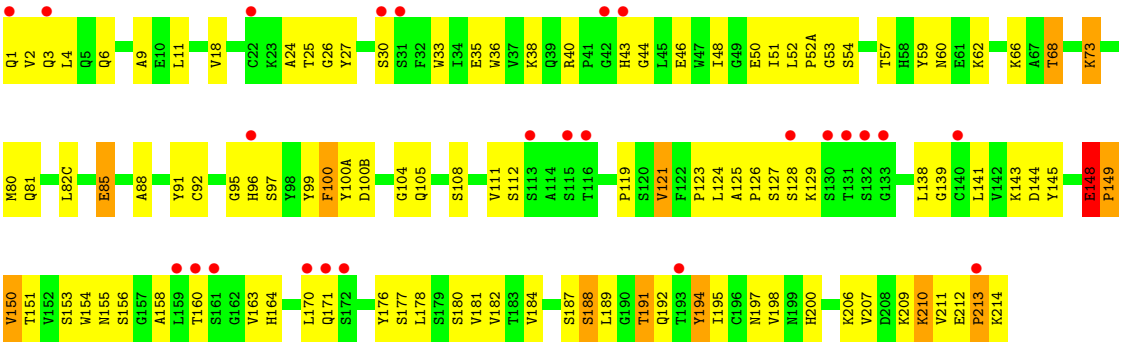
• Molecule 1: chimeric OXY-COPE catalytic ANTIBODY AZ-28 (light chain)

Chain L: 6% 40% 52% 8%



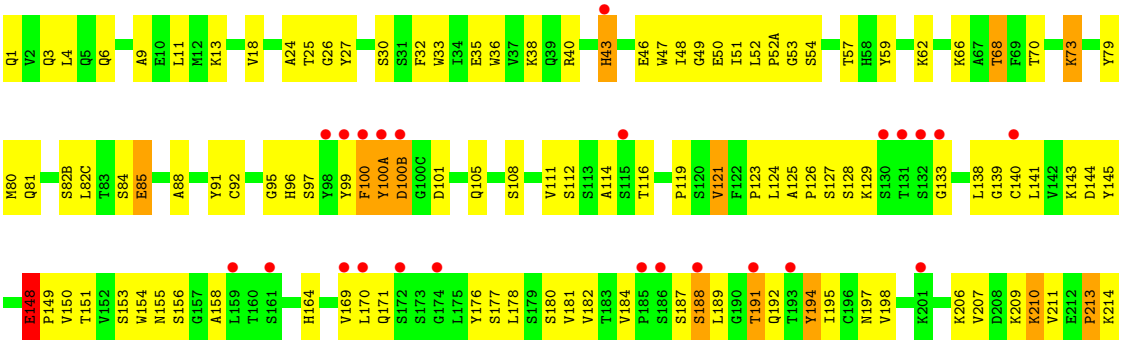
• Molecule 2: chimeric OXY-COPE catalytic ANTIBODY AZ-28 (HEAVY chain)

Chain B: 11% 51% 43% 5%



- Molecule 2: chimeric OXY-COPE catalytic ANTIBODY AZ-28 (HEAVY chain)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.42Å 80.67Å 134.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.2 (20.00-2.80) 87.5 (19.95-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.79Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.232 , 0.285 0.249 , 0.299	Depositor DCC
R_{free} test set	1848 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 86.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6717	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9430e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.52	1/1692 (0.1%)	0.72	1/2290 (0.0%)
1	L	0.56	3/1692 (0.2%)	0.74	2/2290 (0.1%)
2	B	0.44	0/1711	0.73	1/2326 (0.0%)
2	H	0.53	0/1711	0.79	2/2326 (0.1%)
All	All	0.52	4/6806 (0.1%)	0.74	6/9232 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	79	GLU	CG-CD	5.67	1.60	1.51
1	L	143	GLU	CD-OE2	-5.35	1.19	1.25
1	A	143	GLU	CB-CG	5.26	1.62	1.52
1	L	79	GLU	CB-CG	5.02	1.61	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	GLU	OE1-CD-OE2	-6.29	115.75	123.30
2	H	148	GLU	N-CA-C	6.00	127.21	111.00
2	B	148	GLU	N-CA-C	5.81	126.69	111.00
1	L	143	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	L	79	GLU	OE1-CD-OE2	-5.41	116.81	123.30
2	H	100(A)	TYR	CB-CG-CD2	-5.08	117.95	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1656	0	1607	153	0
1	L	1656	0	1607	142	0
2	B	1665	0	1609	122	0
2	H	1665	0	1609	129	0
3	A	1	0	0	0	0
4	A	26	0	0	9	0
4	B	13	0	0	1	0
4	H	17	0	0	6	0
4	L	18	0	0	10	0
All	All	6717	0	6432	518	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:TYR:CD2	1:A:168:SER:HB3	1.84	1.11
1:A:150:VAL:HG23	1:A:151:ASP:H	1.06	1.10
1:A:80:TYR:HD2	1:A:168:SER:HB3	1.07	1.10
1:L:150:VAL:HG23	1:L:151:ASP:H	1.09	1.08
1:L:185:ASP:HA	1:L:188:LYS:HD3	1.42	1.00
1:A:185:ASP:HA	1:A:188:LYS:HD3	1.41	0.99
2:B:126:PRO:HG3	2:B:189:LEU:HD11	1.44	0.99
2:H:126:PRO:HG3	2:H:189:LEU:HD11	1.45	0.99
2:B:1:GLN:N	2:H:13:LYS:HE2	1.81	0.95
1:A:181:LEU:HD13	1:A:186:TYR:HB2	1.47	0.94
1:L:181:LEU:HD13	1:L:186:TYR:HB2	1.48	0.92
2:H:30:SER:HA	2:H:52(A):PRO:HG2	1.51	0.90
1:A:150:VAL:HG23	1:A:151:ASP:N	1.88	0.89
2:B:127:SER:HA	2:B:214:LYS:HB3	1.58	0.86
1:L:150:VAL:HG23	1:L:151:ASP:N	1.90	0.86
2:H:100:PHE:HE1	2:H:100(B):ASP:HB3	1.39	0.85
1:A:201:LEU:HD13	1:A:205:VAL:HG12	1.56	0.84
2:H:191:THR:HG23	2:H:192:GLN:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:201:LEU:HD13	1:L:205:VAL:HG12	1.57	0.83
2:H:100:PHE:CE1	2:H:100(B):ASP:HB3	2.13	0.83
1:L:143:GLU:OE1	4:L:229:HOH:O	1.96	0.83
1:L:28:ASP:OD2	4:L:213:HOH:O	1.96	0.83
1:L:158:ASN:ND2	1:L:179:LEU:HD21	1.94	0.82
2:B:191:THR:HG23	2:B:192:GLN:H	1.42	0.82
1:A:158:ASN:ND2	1:A:179:LEU:HD21	1.96	0.81
2:H:36:TRP:HB3	2:H:80:MET:HE2	1.62	0.81
2:B:36:TRP:HB3	2:B:80:MET:HE2	1.63	0.81
1:A:15:LEU:HD11	1:A:106:ILE:HD13	1.63	0.80
1:A:143:GLU:OE2	4:A:218:HOH:O	2.00	0.80
1:L:198:HIS:CD2	1:L:200:GLY:H	2.00	0.79
1:A:40:PRO:CG	1:A:165:GLU:HG3	2.13	0.78
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.65	0.78
1:A:150:VAL:O	1:A:191:VAL:HG13	1.84	0.78
1:L:193:ALA:HA	1:L:208:SER:HB3	1.65	0.77
1:A:198:HIS:CD2	1:A:200:GLY:H	2.03	0.77
1:A:52:ASN:HA	1:A:64:GLY:HA3	1.67	0.77
2:H:148:GLU:HG2	2:H:176:TYR:CZ	2.20	0.76
1:A:193:ALA:HA	1:A:208:SER:HB3	1.66	0.76
2:B:198:VAL:HG22	2:B:207:VAL:HB	1.67	0.75
2:H:11:LEU:HD23	2:H:116:THR:HG22	1.68	0.75
2:H:195:ILE:HD13	2:H:197:ASN:HD21	1.51	0.75
1:L:80:TYR:HD2	1:L:168:SER:HB3	1.50	0.75
1:L:155:GLN:HB3	1:L:158:ASN:OD1	1.85	0.75
2:B:148:GLU:HG2	2:B:176:TYR:CZ	2.22	0.75
2:B:1:GLN:H1	2:H:13:LYS:HE2	1.48	0.74
1:L:135:LEU:HD11	2:H:181:VAL:HG21	1.69	0.74
2:B:9:ALA:HB1	2:B:149:PRO:HG2	1.68	0.74
1:A:155:GLN:HB3	1:A:158:ASN:OD1	1.87	0.74
1:L:79:GLU:OE2	4:L:215:HOH:O	2.04	0.74
1:L:150:VAL:O	1:L:191:VAL:HG13	1.87	0.74
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.69	0.74
2:H:198:VAL:HG22	2:H:207:VAL:HB	1.69	0.74
2:B:195:ILE:HD13	2:B:197:ASN:HD21	1.51	0.73
1:A:143:GLU:CD	4:A:218:HOH:O	2.27	0.73
1:A:80:TYR:HD2	1:A:168:SER:CB	1.96	0.73
1:L:143:GLU:OE2	4:L:216:HOH:O	2.05	0.73
1:L:139:PHE:HE2	1:L:142:ARG:HA	1.53	0.73
1:A:139:PHE:HE2	1:A:142:ARG:HA	1.54	0.73
1:L:52:ASN:HA	1:L:64:GLY:HA3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:ASN:HD21	1:L:179:LEU:HD21	1.53	0.72
2:H:143:LYS:HD2	2:H:177:SER:OG	1.89	0.72
2:B:1:GLN:H2	2:H:13:LYS:HE2	1.52	0.72
1:A:142:ARG:HB3	1:A:173:TYR:CG	2.25	0.72
1:L:152:ASN:HD22	1:L:152:ASN:N	1.88	0.72
2:B:129:LYS:HB2	4:B:223:HOH:O	1.89	0.71
2:H:100:PHE:HE1	2:H:100(B):ASP:CB	2.04	0.71
2:B:6:GLN:H	2:B:105:GLN:HE22	1.39	0.70
1:L:142:ARG:HB3	1:L:173:TYR:CG	2.26	0.70
1:A:28:ASP:OD2	4:A:213:HOH:O	2.08	0.70
1:A:158:ASN:HD21	1:A:179:LEU:HD21	1.55	0.70
1:A:123:GLU:O	1:A:126:LYS:HG2	1.92	0.70
2:H:126:PRO:HG2	2:H:213:PRO:HB3	1.72	0.69
1:L:192:TYR:O	1:L:208:SER:HB2	1.91	0.69
1:A:117:ILE:HG22	2:B:129:LYS:HE3	1.74	0.69
1:A:142:ARG:O	1:A:144:ALA:N	2.25	0.69
1:A:181:LEU:CD1	1:A:186:TYR:HB2	2.21	0.69
1:L:117:ILE:HG22	2:H:129:LYS:HE3	1.73	0.68
2:B:52:LEU:HD12	2:B:54:SER:H	1.57	0.68
1:L:181:LEU:CD1	1:L:186:TYR:HB2	2.22	0.68
2:H:52:LEU:HD12	2:H:54:SER:H	1.59	0.68
1:A:40:PRO:HG2	1:A:165:GLU:HG3	1.75	0.67
1:L:125:LEU:HD21	1:L:130:ALA:HB2	1.76	0.67
2:B:30:SER:HA	2:B:52(A):PRO:HG2	1.76	0.67
2:B:143:LYS:HD2	2:B:177:SER:OG	1.94	0.67
1:L:142:ARG:O	1:L:144:ALA:N	2.25	0.67
2:B:73:LYS:H	2:B:73:LYS:HZ2	1.42	0.67
1:A:152:ASN:N	1:A:152:ASN:HD22	1.92	0.67
1:L:46:THR:HG22	1:L:55:VAL:HG21	1.75	0.67
1:A:115:VAL:O	1:A:207:LYS:HE3	1.94	0.67
1:L:131:SER:HB3	1:L:180:THR:HG23	1.75	0.67
2:H:73:LYS:CE	2:H:73:LYS:H	2.07	0.67
2:H:127:SER:O	2:H:129:LYS:N	2.28	0.67
2:B:1:GLN:O	2:B:26:GLY:HA3	1.95	0.66
1:A:139:PHE:CE2	1:A:142:ARG:HA	2.30	0.66
1:A:125:LEU:HD21	1:A:130:ALA:HB2	1.77	0.66
1:L:150:VAL:HG22	1:L:155:GLN:HE22	1.60	0.66
1:A:131:SER:HB3	1:A:180:THR:HG23	1.76	0.66
2:B:96:HIS:HB3	2:B:100(A):TYR:CD1	2.30	0.66
1:A:192:TYR:HB2	1:A:209:PHE:CE2	2.30	0.65
1:A:192:TYR:O	1:A:208:SER:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:HG22	1:A:55:VAL:HG21	1.78	0.65
1:L:123:GLU:O	1:L:126:LYS:HG2	1.97	0.65
2:H:133:GLY:HA3	4:H:221:HOH:O	1.96	0.65
1:L:139:PHE:CE2	1:L:142:ARG:HA	2.31	0.65
1:A:119:PRO:HB3	1:A:209:PHE:CE1	2.31	0.65
1:A:150:VAL:HG22	1:A:155:GLN:HE22	1.61	0.65
2:B:68:THR:HG23	2:B:81:GLN:HB3	1.79	0.65
1:L:167:ASP:OD1	4:L:212:HOH:O	2.14	0.65
1:A:12:TYR:CD2	1:A:105:GLU:HB2	2.32	0.64
1:A:15:LEU:CD1	1:A:106:ILE:HD13	2.27	0.64
1:A:17:GLU:OE2	4:A:219:HOH:O	2.14	0.64
2:H:126:PRO:HD3	2:H:138:LEU:HB3	1.77	0.64
2:B:195:ILE:HD12	2:B:195:ILE:O	1.98	0.64
2:H:73:LYS:H	2:H:73:LYS:NZ	1.95	0.64
2:B:73:LYS:H	2:B:73:LYS:NZ	1.95	0.64
1:L:117:ILE:HD13	1:L:208:SER:HA	1.80	0.64
2:B:36:TRP:CB	2:B:80:MET:HE2	2.28	0.64
1:A:150:VAL:CG2	1:A:151:ASP:H	1.90	0.64
1:L:211:ARG:HA	1:L:211:ARG:NH1	2.12	0.64
2:B:126:PRO:HD3	2:B:138:LEU:HB3	1.78	0.63
1:L:79:GLU:OE1	4:L:215:HOH:O	2.15	0.63
2:B:126:PRO:CG	2:B:189:LEU:HD11	2.26	0.63
1:L:149:LYS:HG2	1:L:152:ASN:HA	1.81	0.63
2:B:6:GLN:HB2	2:B:105:GLN:NE2	2.14	0.63
1:A:125:LEU:C	1:A:127:SER:H	2.01	0.63
1:L:125:LEU:CD2	1:L:130:ALA:HB2	2.28	0.63
1:A:135:LEU:HD11	2:B:181:VAL:HG21	1.80	0.63
1:A:149:LYS:HG2	1:A:152:ASN:HA	1.80	0.63
2:B:127:SER:O	2:B:129:LYS:N	2.30	0.62
2:H:214:LYS:O	2:H:214:LYS:HG2	1.99	0.62
1:L:115:VAL:O	1:L:207:LYS:HE3	1.99	0.62
2:B:195:ILE:HG22	2:B:210:LYS:HA	1.80	0.62
2:H:170:LEU:HD23	2:H:176:TYR:CE1	2.34	0.62
1:L:125:LEU:C	1:L:127:SER:H	2.02	0.62
2:H:36:TRP:CB	2:H:80:MET:HE2	2.28	0.62
2:H:195:ILE:HD12	2:H:195:ILE:O	2.00	0.62
2:H:125:ALA:HB1	2:H:213:PRO:HA	1.80	0.62
2:H:195:ILE:HG22	2:H:210:LYS:HA	1.82	0.62
2:B:73:LYS:H	2:B:73:LYS:CE	2.12	0.61
1:L:169:LYS:O	1:L:169:LYS:HD3	1.99	0.61
2:H:18:VAL:HG23	4:H:224:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:THR:HG23	2:H:81:GLN:HB3	1.80	0.61
1:A:28:ASP:OD1	1:A:68:GLY:HA2	2.00	0.61
1:L:211:ARG:HA	1:L:211:ARG:HH11	1.64	0.61
2:B:18:VAL:HG12	2:B:82(C):LEU:HD21	1.82	0.61
2:H:148:GLU:HG2	2:H:176:TYR:CE1	2.34	0.60
2:H:73:LYS:HB2	2:H:73:LYS:HZ2	1.66	0.60
1:A:125:LEU:CD2	1:A:130:ALA:HB2	2.31	0.60
2:B:6:GLN:N	2:B:105:GLN:HE22	2.00	0.60
1:L:152:ASN:HD22	1:L:152:ASN:H	1.48	0.60
2:H:209:LYS:HG3	2:H:210:LYS:N	2.17	0.60
1:A:117:ILE:HD13	1:A:208:SER:HA	1.84	0.59
1:A:169:LYS:O	1:A:169:LYS:HD3	2.01	0.59
1:L:21:ILE:HG13	1:L:73:LEU:HB3	1.83	0.59
1:A:21:ILE:HG13	1:A:73:LEU:HB3	1.85	0.59
2:H:6:GLN:H	2:H:105:GLN:HE22	1.49	0.59
2:H:126:PRO:CG	2:H:189:LEU:HD11	2.27	0.59
2:B:155:ASN:OD1	2:B:194:TYR:HA	2.03	0.59
1:A:125:LEU:HD22	1:A:183:LYS:HG3	1.83	0.59
1:L:73:LEU:C	1:L:73:LEU:HD23	2.22	0.59
2:B:148:GLU:HG2	2:B:176:TYR:CE1	2.38	0.59
1:L:198:HIS:HD2	1:L:200:GLY:H	1.50	0.59
2:B:170:LEU:HD23	2:B:176:TYR:CE1	2.37	0.59
2:B:127:SER:HA	2:B:214:LYS:CB	2.32	0.58
1:L:28:ASP:OD1	1:L:68:GLY:HA2	2.02	0.58
2:H:35:GLU:O	2:H:92:CYS:HA	2.03	0.58
1:A:123:GLU:OE2	2:B:209:LYS:HE3	2.03	0.58
1:L:125:LEU:HD22	1:L:183:LYS:HG3	1.84	0.58
2:B:73:LYS:HB2	2:B:73:LYS:HZ3	1.67	0.58
2:B:73:LYS:HZ2	2:B:73:LYS:N	2.00	0.58
1:L:197:THR:HG22	1:L:204:PRO:HG3	1.85	0.58
1:L:18:ARG:HG3	1:L:76:SER:HA	1.86	0.58
1:L:193:ALA:HA	1:L:208:SER:CB	2.32	0.58
1:A:73:LEU:C	1:A:73:LEU:HD23	2.24	0.58
1:A:197:THR:HG22	1:A:204:PRO:HG3	1.86	0.58
1:A:152:ASN:HD22	1:A:152:ASN:H	1.50	0.57
1:A:85:ILE:HD13	1:A:103:LYS:HG3	1.86	0.57
1:L:123:GLU:OE2	2:H:209:LYS:HE3	2.05	0.57
1:A:5:THR:O	1:A:23:CYS:HA	2.04	0.57
2:B:9:ALA:CB	2:B:149:PRO:HG2	2.34	0.57
1:L:28:ASP:OD2	1:L:30:ASN:OD1	2.23	0.57
2:H:155:ASN:OD1	2:H:194:TYR:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:VAL:HG12	1:L:75:ILE:HB	1.87	0.56
1:A:201:LEU:HD13	1:A:205:VAL:CG1	2.33	0.56
2:B:35:GLU:O	2:B:92:CYS:HA	2.04	0.56
2:H:96:HIS:HB3	2:H:100(A):TYR:CD1	2.40	0.56
1:A:144:ALA:HB2	1:A:198:HIS:ND1	2.19	0.56
1:L:79:GLU:CD	4:L:215:HOH:O	2.43	0.56
2:H:73:LYS:H	2:H:73:LYS:HE3	1.70	0.56
2:H:195:ILE:CD1	2:H:197:ASN:HD21	2.17	0.56
2:H:97:SER:C	2:H:99:TYR:H	2.08	0.56
1:A:193:ALA:HA	1:A:208:SER:CB	2.34	0.56
2:B:211:VAL:O	2:B:211:VAL:HG13	2.05	0.56
1:A:7:SER:HA	1:A:8:PRO:C	2.26	0.56
1:A:18:ARG:HG3	1:A:76:SER:HA	1.86	0.56
1:L:22:THR:HG22	1:L:72:SER:HB3	1.88	0.56
1:L:40:PRO:CG	1:L:165:GLU:HG3	2.36	0.56
1:L:121:SER:OG	2:H:123:PRO:HD2	2.03	0.56
1:L:201:LEU:HD13	1:L:205:VAL:CG1	2.34	0.56
2:B:209:LYS:HG3	2:B:210:LYS:N	2.21	0.55
1:A:117:ILE:O	2:B:129:LYS:HE2	2.06	0.55
2:B:82(C):LEU:HB3	2:B:111:VAL:HG22	1.87	0.55
1:A:22:THR:HG22	1:A:72:SER:HB3	1.89	0.55
1:L:144:ALA:HB2	1:L:198:HIS:ND1	2.21	0.55
2:H:112:SER:C	2:H:114:ALA:H	2.10	0.55
2:B:57:THR:HG1	2:B:59:TYR:HE2	1.53	0.55
2:B:141:LEU:HD21	2:B:143:LYS:HD3	1.88	0.55
2:B:46:GLU:OE2	2:B:62:LYS:NZ	2.40	0.55
2:H:46:GLU:OE2	2:H:62:LYS:NZ	2.40	0.55
1:A:142:ARG:NH2	1:A:163:VAL:HB	2.22	0.55
1:A:19:VAL:HG12	1:A:75:ILE:HB	1.89	0.54
1:A:198:HIS:HD2	1:A:200:GLY:H	1.54	0.54
1:L:5:THR:O	1:L:23:CYS:HA	2.07	0.54
2:H:127:SER:C	2:H:129:LYS:H	2.11	0.54
1:A:175:LEU:C	1:A:175:LEU:HD23	2.28	0.54
1:A:52:ASN:HB3	1:A:64:GLY:O	2.08	0.54
1:L:146:VAL:HB	1:L:161:GLU:OE2	2.07	0.54
2:H:182:VAL:HG22	2:H:184:VAL:HG13	1.90	0.54
1:A:125:LEU:C	1:A:127:SER:N	2.61	0.54
1:A:39:LYS:HE3	1:A:83:MET:O	2.08	0.54
1:L:142:ARG:NH2	1:L:163:VAL:HB	2.23	0.54
2:H:153:SER:O	2:H:197:ASN:N	2.37	0.54
1:A:17:GLU:CD	4:A:219:HOH:O	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:OE2	2:B:123:PRO:HD3	2.09	0.53
2:B:3:GLN:O	2:B:4:LEU:HG	2.08	0.53
2:B:195:ILE:CD1	2:B:197:ASN:HD21	2.19	0.53
1:L:150:VAL:HG22	1:L:155:GLN:NE2	2.23	0.53
1:L:137:ASN:HD21	2:H:164:HIS:CD2	2.25	0.53
2:B:82(C):LEU:HB3	2:B:111:VAL:CG2	2.39	0.53
1:L:80:TYR:CD2	1:L:168:SER:HB3	2.39	0.53
2:H:35:GLU:HG2	2:H:50:GLU:HB3	1.90	0.53
2:B:9:ALA:HB1	2:B:108:SER:HB3	1.91	0.53
1:L:7:SER:HA	1:L:8:PRO:C	2.27	0.53
2:H:123:PRO:CB	2:H:211:VAL:HG22	2.38	0.53
1:A:146:VAL:HB	1:A:161:GLU:OE2	2.08	0.53
2:B:124:LEU:HB2	2:B:139:GLY:O	2.09	0.53
1:A:150:VAL:HG22	1:A:155:GLN:NE2	2.23	0.53
2:H:129:LYS:HB2	4:H:228:HOH:O	2.09	0.53
2:B:2:VAL:HA	2:B:25:THR:O	2.09	0.53
1:L:14:SER:OG	1:L:17:GLU:HG3	2.08	0.53
1:L:117:ILE:CD1	1:L:208:SER:HA	2.39	0.53
1:L:151:ASP:OD1	1:L:191:VAL:HG12	2.08	0.53
1:L:175:LEU:HD23	1:L:175:LEU:C	2.29	0.53
1:L:125:LEU:C	1:L:127:SER:N	2.61	0.52
1:L:143:GLU:CD	4:L:216:HOH:O	2.45	0.52
2:H:3:GLN:O	2:H:4:LEU:HG	2.08	0.52
1:A:66:GLY:HA3	1:A:71:TYR:HA	1.91	0.52
1:A:151:ASP:OD1	1:A:191:VAL:HG12	2.09	0.52
2:B:143:LYS:NZ	2:B:171:GLN:HE22	2.06	0.52
1:A:152:ASN:N	1:A:152:ASN:ND2	2.58	0.52
2:B:127:SER:C	2:B:129:LYS:H	2.13	0.52
1:L:150:VAL:CG2	1:L:151:ASP:H	1.93	0.52
2:B:182:VAL:HG22	2:B:184:VAL:HG13	1.92	0.52
1:A:14:SER:OG	1:A:17:GLU:HG3	2.10	0.52
1:L:110:VAL:HG12	1:L:111:ALA:N	2.25	0.52
1:L:150:VAL:HG12	1:L:192:TYR:CE1	2.45	0.51
1:A:122:ASP:OD2	1:A:123:GLU:N	2.42	0.51
2:B:153:SER:O	2:B:197:ASN:N	2.39	0.51
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.92	0.51
1:A:87:TYR:OH	2:B:44:GLY:HA2	2.11	0.51
2:B:73:LYS:H	2:B:73:LYS:HE3	1.76	0.51
1:L:54:LEU:HD21	1:L:62:PHE:O	2.10	0.51
1:L:91:TYR:HA	1:L:96:TYR:CD1	2.45	0.51
1:L:158:ASN:ND2	1:L:179:LEU:CD2	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:THR:HG1	2:H:59:TYR:HE2	1.59	0.51
2:H:143:LYS:NZ	2:H:171:GLN:HE22	2.08	0.51
1:A:15:LEU:HD11	1:A:106:ILE:CD1	2.38	0.51
2:B:195:ILE:HG22	2:B:209:LYS:O	2.11	0.51
1:L:152:ASN:N	1:L:152:ASN:ND2	2.56	0.51
1:A:91:TYR:HA	1:A:96:TYR:CD1	2.46	0.51
2:B:52:LEU:CD1	2:B:54:SER:H	2.21	0.50
2:B:139:GLY:HA2	2:B:154:TRP:CZ2	2.46	0.50
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.93	0.50
2:B:11:LEU:HD11	2:B:112:SER:HB3	1.94	0.50
1:L:4:MET:O	1:L:99:GLY:HA2	2.12	0.50
1:A:54:LEU:HD21	1:A:62:PHE:O	2.11	0.50
1:A:121:SER:OG	2:B:123:PRO:HD2	2.12	0.50
1:L:120:PRO:HG2	1:L:186:TYR:CZ	2.46	0.50
2:B:100:PHE:HZ	2:B:100(B):ASP:OD2	1.95	0.50
1:A:167:ASP:OD1	1:A:169:LYS:HB3	2.11	0.50
2:B:143:LYS:HZ3	2:B:171:GLN:CD	2.11	0.50
1:L:170:ASP:N	1:L:170:ASP:OD1	2.45	0.50
2:H:139:GLY:HA3	2:H:181:VAL:HA	1.93	0.50
1:A:110:VAL:HG12	1:A:111:ALA:N	2.27	0.50
2:H:32:PHE:CD1	2:H:97:SER:HB3	2.46	0.50
2:H:52:LEU:CD1	2:H:54:SER:H	2.23	0.50
2:H:139:GLY:HA2	2:H:154:TRP:CZ2	2.46	0.50
2:H:143:LYS:HZ3	2:H:171:GLN:CD	2.10	0.50
1:A:34:ASN:OD1	1:A:49:TYR:HA	2.12	0.50
1:A:120:PRO:HG2	1:A:186:TYR:CZ	2.47	0.50
2:H:141:LEU:HD21	2:H:143:LYS:HD3	1.93	0.50
1:L:21:ILE:HD11	1:L:73:LEU:HD22	1.94	0.49
1:A:21:ILE:O	1:A:72:SER:HB2	2.11	0.49
2:B:24:ALA:HB1	2:B:27:TYR:CE1	2.47	0.49
1:A:3:LYS:HE2	1:A:5:THR:OG1	2.12	0.49
1:L:34:ASN:OD1	1:L:49:TYR:HA	2.12	0.49
1:L:123:GLU:OE2	2:H:123:PRO:HD3	2.11	0.49
2:H:36:TRP:O	2:H:48:ILE:HB	2.12	0.49
2:B:35:GLU:HG2	2:B:50:GLU:HB3	1.94	0.49
2:H:9:ALA:HB1	2:H:108:SER:HB3	1.94	0.49
2:H:38:LYS:HE2	2:H:40:ARG:HG3	1.94	0.49
1:A:175:LEU:HD23	1:A:176:SER:N	2.28	0.49
2:H:195:ILE:HG22	2:H:209:LYS:O	2.12	0.49
2:B:33:TRP:HD1	2:B:96:HIS:O	1.96	0.49
2:B:139:GLY:HA3	2:B:181:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HB2	2:B:60:ASN:ND2	2.27	0.49
1:A:117:ILE:CD1	1:A:208:SER:HA	2.42	0.49
1:L:52:ASN:HB3	1:L:64:GLY:O	2.13	0.49
2:H:124:LEU:HB2	2:H:139:GLY:O	2.12	0.49
1:A:150:VAL:HG12	1:A:192:TYR:CE1	2.48	0.49
1:L:21:ILE:O	1:L:72:SER:HB2	2.12	0.49
1:L:39:LYS:HE3	1:L:83:MET:O	2.13	0.49
1:L:105:GLU:OE1	1:L:173:TYR:OH	2.26	0.49
2:H:100(B):ASP:OD1	2:H:100(B):ASP:O	2.31	0.49
1:A:112:ALA:HB1	1:A:201:LEU:CD2	2.43	0.48
1:L:137:ASN:ND2	2:H:164:HIS:CD2	2.81	0.48
1:L:3:LYS:HE2	1:L:5:THR:OG1	2.12	0.48
1:L:143:GLU:CD	4:L:229:HOH:O	2.47	0.48
1:A:28:ASP:C	1:A:30:ASN:H	2.16	0.48
2:H:6:GLN:N	2:H:105:GLN:HE22	2.10	0.48
2:B:4:LEU:HD23	2:B:24:ALA:HA	1.95	0.48
2:B:126:PRO:HD3	2:B:138:LEU:CB	2.42	0.48
1:L:122:ASP:OD2	1:L:123:GLU:N	2.43	0.48
2:H:43:HIS:CD2	4:H:229:HOH:O	2.65	0.48
2:B:214:LYS:HB2	2:B:214:LYS:HE3	1.70	0.48
1:L:17:GLU:OE2	4:L:221:HOH:O	2.19	0.48
2:H:178:LEU:HD12	2:H:178:LEU:C	2.34	0.48
1:A:6:GLN:OE1	1:A:101:GLY:N	2.47	0.48
1:L:93:GLU:HG2	1:L:94:PHE:N	2.29	0.48
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.95	0.48
1:A:20:THR:HB	1:A:74:THR:OG1	2.14	0.48
1:A:21:ILE:HD11	1:A:73:LEU:HD22	1.96	0.48
2:B:36:TRP:CZ3	2:B:92:CYS:HB3	2.49	0.48
2:B:97:SER:C	2:B:99:TYR:H	2.16	0.48
1:L:91:TYR:CZ	2:H:100(A):TYR:HE2	2.32	0.48
1:A:170:ASP:OD1	1:A:170:ASP:N	2.46	0.47
2:B:195:ILE:HD13	2:B:197:ASN:ND2	2.26	0.47
1:L:28:ASP:C	1:L:30:ASN:H	2.16	0.47
1:L:149:LYS:CG	1:L:152:ASN:HA	2.44	0.47
2:B:1:GLN:H1	2:H:13:LYS:CE	2.23	0.47
1:A:149:LYS:CG	1:A:152:ASN:HA	2.43	0.47
1:L:46:THR:HG22	1:L:55:VAL:CG2	2.44	0.47
2:H:6:GLN:HB2	2:H:105:GLN:NE2	2.29	0.47
2:H:82(C):LEU:HB3	2:H:111:VAL:CG2	2.45	0.47
1:A:80:TYR:CE2	1:A:168:SER:HB3	2.41	0.47
1:L:112:ALA:HB1	1:L:201:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:ASP:OD1	1:L:169:LYS:HB3	2.14	0.47
2:H:25:THR:CG2	2:H:26:GLY:N	2.78	0.47
2:H:123:PRO:HB2	2:H:211:VAL:HG22	1.97	0.47
1:A:141:PRO:O	1:A:198:HIS:HE1	1.97	0.47
2:B:25:THR:CG2	2:B:26:GLY:N	2.78	0.47
1:L:110:VAL:CG1	1:L:111:ALA:N	2.78	0.47
1:L:150:VAL:H	1:L:155:GLN:HE21	1.63	0.47
2:B:178:LEU:C	2:B:178:LEU:HD12	2.35	0.47
2:B:125:ALA:CB	2:B:212:GLU:O	2.63	0.46
1:L:46:THR:OG1	2:H:101:ASP:HB2	2.15	0.46
2:H:11:LEU:HD11	2:H:112:SER:HB3	1.96	0.46
1:A:33:LEU:HA	1:A:89:LEU:O	2.14	0.46
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.49	0.46
1:A:4:MET:O	1:A:99:GLY:HA2	2.15	0.46
1:L:141:PRO:O	1:L:198:HIS:HE1	1.98	0.46
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.97	0.46
2:H:40:ARG:HG2	2:H:88:ALA:HB2	1.97	0.46
2:H:126:PRO:HD3	2:H:138:LEU:CB	2.43	0.46
1:A:28:ASP:OD2	1:A:30:ASN:OD1	2.33	0.46
2:B:38:LYS:HE2	2:B:40:ARG:HG3	1.98	0.46
2:B:187:SER:OG	2:B:188:SER:N	2.49	0.46
2:H:51:ILE:HB	2:H:57:THR:HG22	1.97	0.46
1:A:61:ARG:CB	1:A:76:SER:OG	2.64	0.46
1:A:93:GLU:HG2	1:A:94:PHE:N	2.29	0.46
2:B:6:GLN:HE22	2:B:91:TYR:HA	1.80	0.46
2:H:194:TYR:CD1	2:H:194:TYR:N	2.83	0.46
1:A:56:ASP:OD1	2:H:84:SER:HA	2.15	0.46
1:A:201:LEU:C	1:A:203:SER:H	2.18	0.46
2:H:187:SER:OG	2:H:188:SER:N	2.48	0.46
1:A:150:VAL:H	1:A:155:GLN:HE21	1.64	0.46
1:L:201:LEU:C	1:L:203:SER:H	2.18	0.46
1:A:40:PRO:CB	1:A:165:GLU:HG3	2.46	0.46
1:L:6:GLN:OE1	1:L:101:GLY:N	2.49	0.46
1:L:175:LEU:HD23	1:L:176:SER:N	2.31	0.46
1:L:33:LEU:HD13	1:L:71:TYR:CG	2.51	0.45
2:B:121:VAL:O	2:B:121:VAL:HG22	2.16	0.45
1:L:106:ILE:HD12	1:L:171:SER:OG	2.16	0.45
1:L:191:VAL:HG22	1:L:192:TYR:N	2.32	0.45
2:H:66:LYS:NZ	2:H:82(B):SER:O	2.49	0.45
2:B:36:TRP:O	2:B:48:ILE:HB	2.16	0.45
2:B:153:SER:HB2	2:B:197:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TRP:CE2	1:A:179:LEU:HB2	2.51	0.45
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.51	0.45
1:A:61:ARG:HB3	1:A:76:SER:OG	2.16	0.45
2:H:6:GLN:HE22	2:H:91:TYR:HA	1.82	0.45
2:H:11:LEU:CD2	2:H:116:THR:HG22	2.41	0.45
1:A:158:ASN:ND2	1:A:179:LEU:CD2	2.74	0.45
2:B:139:GLY:HA2	2:B:154:TRP:CH2	2.52	0.45
2:B:9:ALA:CB	2:B:108:SER:HB3	2.46	0.45
2:B:108:SER:OG	2:B:149:PRO:HG3	2.16	0.45
1:L:117:ILE:O	2:H:129:LYS:HE2	2.17	0.45
2:H:125:ALA:HB1	2:H:213:PRO:CA	2.47	0.45
1:A:46:THR:HG22	1:A:55:VAL:CG2	2.46	0.44
1:A:71:TYR:N	1:A:71:TYR:CD1	2.85	0.44
1:A:142:ARG:HD3	4:A:238:HOH:O	2.15	0.44
2:B:191:THR:HG23	2:B:192:GLN:N	2.22	0.44
1:L:27:GLN:O	1:L:29:ILE:N	2.50	0.44
1:L:90:GLN:CD	1:L:90:GLN:O	2.56	0.44
2:H:195:ILE:HD13	2:H:197:ASN:ND2	2.26	0.44
2:H:36:TRP:HA	2:H:91:TYR:O	2.17	0.44
2:H:100(B):ASP:O	2:H:100(B):ASP:CG	2.56	0.44
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.16	0.44
1:A:90:GLN:O	1:A:90:GLN:CD	2.55	0.44
1:A:179:LEU:HD22	1:A:179:LEU:HA	1.77	0.44
2:B:138:LEU:HG	2:B:182:VAL:HG13	1.98	0.44
2:H:169:VAL:O	2:H:169:VAL:HG23	2.18	0.44
2:B:36:TRP:HA	2:B:91:TYR:O	2.18	0.44
2:B:150:VAL:HG23	2:B:200:HIS:HB2	1.99	0.44
2:B:51:ILE:HB	2:B:57:THR:HG22	1.99	0.44
1:A:17:GLU:OE1	4:A:219:HOH:O	2.21	0.44
2:B:138:LEU:HD21	2:B:194:TYR:CE1	2.53	0.44
1:A:33:LEU:HD13	1:A:71:TYR:CG	2.53	0.43
1:A:110:VAL:CG1	1:A:111:ALA:N	2.80	0.43
1:A:137:ASN:HD21	2:B:164:HIS:CD2	2.36	0.43
1:L:61:ARG:CB	1:L:76:SER:OG	2.66	0.43
1:A:198:HIS:CD2	1:A:200:GLY:N	2.80	0.43
2:H:209:LYS:HG3	2:H:210:LYS:H	1.83	0.43
1:L:148:TRP:CE2	1:L:179:LEU:HB2	2.53	0.43
2:H:9:ALA:CB	2:H:108:SER:HB3	2.49	0.43
2:H:85:GLU:CD	2:H:85:GLU:N	2.72	0.43
2:H:138:LEU:HD21	2:H:194:TYR:CE1	2.53	0.43
1:A:201:LEU:C	1:A:203:SER:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:HE21	2:B:104:GLY:HA3	1.83	0.43
1:L:33:LEU:HA	1:L:89:LEU:O	2.18	0.43
1:A:159:SER:HA	1:A:178:THR:O	2.18	0.43
2:H:126:PRO:HB2	2:H:189:LEU:HD21	1.99	0.43
1:L:150:VAL:H	1:L:155:GLN:NE2	2.16	0.43
2:H:121:VAL:HA	2:H:141:LEU:O	2.18	0.43
1:A:209:PHE:N	1:A:209:PHE:CD2	2.86	0.43
2:B:194:TYR:CD1	2:B:194:TYR:N	2.86	0.43
2:B:214:LYS:O	2:B:214:LYS:HG3	2.19	0.43
1:L:159:SER:HA	1:L:178:THR:O	2.19	0.43
2:H:138:LEU:HG	2:H:182:VAL:HG13	2.01	0.43
1:A:15:LEU:CD1	1:A:106:ILE:CD1	2.95	0.43
2:H:30:SER:HB2	2:H:53:GLY:CA	2.49	0.43
2:H:125:ALA:HA	2:H:211:VAL:CG1	2.49	0.43
2:H:209:LYS:HZ3	2:H:210:LYS:HG2	1.84	0.43
2:B:212:GLU:HA	2:B:213:PRO:HD2	1.82	0.42
1:L:2:ILE:HD13	1:L:29:ILE:HG22	2.01	0.42
1:A:191:VAL:HG22	1:A:192:TYR:N	2.34	0.42
2:B:121:VAL:HA	2:B:141:LEU:O	2.19	0.42
2:H:191:THR:HG23	2:H:192:GLN:N	2.22	0.42
1:A:70:ASP:C	1:A:71:TYR:CD1	2.93	0.42
1:L:198:HIS:CD2	1:L:200:GLY:N	2.78	0.42
2:B:1:GLN:C	2:B:26:GLY:HA3	2.40	0.42
2:H:153:SER:HB2	2:H:197:ASN:HB2	2.01	0.42
1:A:169:LYS:HG2	1:L:185:ASP:OD1	2.20	0.42
1:A:2:ILE:HD13	1:A:29:ILE:HG22	2.02	0.42
1:A:195:GLU:CD	4:A:214:HOH:O	2.58	0.42
1:A:209:PHE:HD2	1:A:209:PHE:H	1.66	0.42
1:L:12:TYR:HA	1:L:105:GLU:O	2.20	0.42
1:L:19:VAL:HG21	1:L:104:LEU:HD11	2.01	0.42
1:L:20:THR:HB	1:L:74:THR:OG1	2.19	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.87	0.42
2:B:143:LYS:NZ	2:B:171:GLN:NE2	2.68	0.42
2:B:85:GLU:N	2:B:85:GLU:CD	2.73	0.42
1:L:183:LYS:O	1:L:187:GLU:HG2	2.20	0.42
2:H:129:LYS:CG	4:H:220:HOH:O	2.68	0.42
1:A:85:ILE:CD1	1:A:103:LYS:HG3	2.47	0.42
1:A:149:LYS:HG2	1:A:152:ASN:CA	2.47	0.41
2:B:126:PRO:HB2	2:B:189:LEU:HD21	2.02	0.41
1:L:26:SER:C	1:L:27:GLN:HG2	2.40	0.41
1:L:122:ASP:OD2	1:L:123:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:PHE:CD1	2:H:100:PHE:C	2.93	0.41
1:A:150:VAL:H	1:A:155:GLN:NE2	2.18	0.41
2:B:187:SER:C	2:B:189:LEU:H	2.23	0.41
1:L:13:ALA:HB3	1:L:78:LEU:HD22	2.01	0.41
1:L:31:SER:HA	1:L:71:TYR:CE2	2.55	0.41
1:L:61:ARG:HB3	1:L:76:SER:OG	2.20	0.41
1:L:142:ARG:HB3	1:L:173:TYR:CD2	2.55	0.41
1:A:54:LEU:O	2:H:84:SER:CB	2.69	0.41
1:A:142:ARG:HB3	1:A:173:TYR:CD2	2.53	0.41
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.20	0.41
2:H:121:VAL:O	2:H:121:VAL:HG22	2.20	0.41
1:A:13:ALA:HB3	1:A:78:LEU:HD22	2.01	0.41
1:A:27:GLN:O	1:A:29:ILE:N	2.53	0.41
2:B:119:PRO:CB	2:B:145:TYR:HB3	2.42	0.41
2:B:156:SER:HA	2:B:197:ASN:OD1	2.20	0.41
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.56	0.41
1:A:145:LYS:HG3	4:A:220:HOH:O	2.20	0.41
2:H:143:LYS:NZ	2:H:171:GLN:NE2	2.69	0.41
1:A:31:SER:HA	1:A:71:TYR:CE2	2.55	0.41
2:B:30:SER:HB2	2:B:53:GLY:CA	2.51	0.41
2:B:66:LYS:HA	2:B:66:LYS:HD3	1.84	0.41
1:A:4:MET:HE2	1:A:90:GLN:HB3	2.01	0.41
1:A:137:ASN:ND2	2:B:164:HIS:CD2	2.89	0.41
2:B:40:ARG:HG2	2:B:88:ALA:HB2	2.03	0.41
1:L:40:PRO:HG2	1:L:165:GLU:HG3	2.01	0.41
1:L:149:LYS:HG2	1:L:152:ASN:CA	2.50	0.41
2:H:73:LYS:NZ	2:H:73:LYS:N	2.65	0.41
2:H:156:SER:HA	2:H:197:ASN:OD1	2.21	0.41
2:B:38:LYS:HB2	2:B:48:ILE:HD11	2.03	0.41
2:B:194:TYR:O	2:B:211:VAL:HG12	2.20	0.41
1:L:115:VAL:O	1:L:207:LYS:HG2	2.21	0.41
2:H:33:TRP:HD1	2:H:96:HIS:O	2.03	0.41
2:H:36:TRP:CZ3	2:H:92:CYS:HB3	2.56	0.41
2:H:140:CYS:N	2:H:180:SER:O	2.54	0.41
2:H:177:SER:HB2	4:H:226:HOH:O	2.20	0.41
2:H:187:SER:C	2:H:189:LEU:H	2.24	0.41
1:A:56:ASP:N	2:H:84:SER:HB2	2.36	0.41
1:A:183:LYS:O	1:A:187:GLU:HG2	2.20	0.41
1:L:4:MET:HE2	1:L:90:GLN:HB3	2.02	0.40
1:L:67:SER:HA	1:L:71:TYR:CE2	2.56	0.40
1:A:26:SER:C	1:A:27:GLN:HG2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HB	1:A:205:VAL:HG13	2.03	0.40
1:L:71:TYR:CD1	1:L:71:TYR:N	2.89	0.40
1:L:201:LEU:C	1:L:203:SER:N	2.74	0.40
2:H:70:THR:OG1	2:H:79:TYR:HB2	2.21	0.40
2:H:97:SER:C	2:H:99:TYR:N	2.74	0.40
2:B:160:THR:HG23	2:B:163:VAL:HG21	2.04	0.40
2:B:100:PHE:CZ	2:B:100(B):ASP:OD2	2.74	0.40
2:B:139:GLY:HA3	2:B:180:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/211 (99%)	175 (84%)	27 (13%)	7 (3%)	4	13
1	L	209/211 (99%)	175 (84%)	26 (12%)	8 (4%)	3	10
2	B	219/221 (99%)	188 (86%)	23 (10%)	8 (4%)	3	11
2	H	219/221 (99%)	187 (85%)	24 (11%)	8 (4%)	3	11
All	All	856/864 (99%)	725 (85%)	100 (12%)	31 (4%)	3	11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	150	VAL
2	B	128	SER
1	L	143	GLU
1	L	150	VAL
2	H	128	SER
1	A	28	ASP

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Mol	Chain	Res	Type
1	A	80	TYR
1	A	168	SER
2	B	95	GLY
2	B	144	ASP
2	B	148	GLU
2	B	158	ALA
1	L	28	ASP
1	L	168	SER
2	H	95	GLY
2	H	144	ASP
2	H	148	GLU
2	H	158	ALA
2	H	213	PRO
1	A	155	GLN
2	B	149	PRO
2	B	188	SER
1	L	51	THR
1	L	155	GLN
2	H	188	SER
1	A	51	THR
1	L	80	TYR
2	H	149	PRO
1	L	138	ASN
2	B	213	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/190 (100%)	178 (94%)	12 (6%)	18	46
1	L	190/190 (100%)	178 (94%)	12 (6%)	18	46
2	B	185/185 (100%)	172 (93%)	13 (7%)	15	40
2	H	185/185 (100%)	170 (92%)	15 (8%)	11	33
All	All	750/750 (100%)	698 (93%)	52 (7%)	15	41

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	21	ILE
1	A	74	THR
1	A	83	MET
1	A	127	SER
1	A	135	LEU
1	A	142	ARG
1	A	160	GLN
1	A	171	SER
1	A	181	LEU
1	A	205	VAL
1	A	209	PHE
2	B	43	HIS
2	B	68	THR
2	B	73	LYS
2	B	85	GLU
2	B	100	PHE
2	B	121	VAL
2	B	148	GLU
2	B	150	VAL
2	B	151	THR
2	B	191	THR
2	B	194	TYR
2	B	206	LYS
2	B	210	LYS
1	L	14	SER
1	L	21	ILE
1	L	83	MET
1	L	127	SER
1	L	135	LEU
1	L	142	ARG
1	L	152	ASN
1	L	160	GLN
1	L	171	SER
1	L	181	LEU
1	L	205	VAL
1	L	211	ARG
2	H	1	GLN
2	H	43	HIS
2	H	68	THR
2	H	73	LYS
2	H	85	GLU

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Mol	Chain	Res	Type
2	H	100	PHE
2	H	100(B)	ASP
2	H	121	VAL
2	H	148	GLU
2	H	150	VAL
2	H	151	THR
2	H	191	THR
2	H	194	TYR
2	H	206	LYS
2	H	210	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	137	ASN
1	A	138	ASN
1	A	147	GLN
1	A	152	ASN
1	A	155	GLN
1	A	198	HIS
1	A	199	GLN
2	B	6	GLN
2	B	43	HIS
2	B	58	HIS
2	B	76	ASN
2	B	105	GLN
2	B	164	HIS
2	B	204	ASN
1	L	69	GLN
1	L	137	ASN
1	L	138	ASN
1	L	147	GLN
1	L	152	ASN
1	L	155	GLN
1	L	198	HIS
1	L	199	GLN
2	H	6	GLN
2	H	43	HIS
2	H	58	HIS
2	H	164	HIS
2	H	204	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	211/211 (100%)	0.36	14 (6%)	18	11	20, 51, 88, 95	0
1	L	211/211 (100%)	0.20	12 (5%)	23	15	20, 43, 78, 94	0
2	B	221/221 (100%)	0.54	25 (11%)	5	3	17, 52, 87, 95	0
2	H	221/221 (100%)	0.39	24 (10%)	5	3	11, 44, 86, 95	0
All	All	864/864 (100%)	0.37	75 (8%)	10	5	11, 47, 87, 95	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	130	SER	9.3
2	H	130	SER	8.3
2	H	131	THR	7.0
2	H	133	GLY	5.5
2	B	193	THR	5.2
2	B	128	SER	4.8
2	H	132	SER	4.7
2	B	170	LEU	4.7
2	H	159	LEU	4.5
1	A	157	GLY	4.0
2	B	213	PRO	3.9
2	H	99	TYR	3.9
2	B	115	SER	3.9
2	B	160	THR	3.9
2	B	159	LEU	3.6
2	H	161	SER	3.6
2	B	31	SER	3.5
2	H	100(A)	TYR	3.5
1	A	210	ASN	3.5
2	B	131	THR	3.4
1	L	126	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	43	HIS	3.3
2	B	30	SER	3.3
1	L	153	ALA	3.3
2	B	140	CYS	3.3
2	H	186	SER	3.2
2	B	42	GLY	3.2
2	H	100	PHE	3.2
1	A	156	SER	3.1
2	B	116	THR	3.0
2	B	133	GLY	3.0
1	L	157	GLY	2.9
2	B	171	GLN	2.8
1	A	183	LYS	2.8
1	L	182	SER	2.8
1	A	7	SER	2.7
1	A	191	VAL	2.6
2	H	98	TYR	2.6
2	H	169	VAL	2.6
1	L	24	LYS	2.6
1	A	126	LYS	2.6
2	B	132	SER	2.6
2	H	140	CYS	2.5
1	A	15	LEU	2.5
2	B	22	CYS	2.5
2	B	113	SER	2.4
2	H	172	SER	2.4
1	L	156	SER	2.4
2	H	115	SER	2.4
1	A	154	LEU	2.4
1	L	154	LEU	2.4
2	H	185	PRO	2.4
1	L	57	GLY	2.4
1	A	1	ASP	2.3
1	L	187	GLU	2.3
2	H	100(B)	ASP	2.3
2	B	172	SER	2.3
1	L	169	LYS	2.2
2	H	170	LEU	2.2
2	H	43	HIS	2.2
1	A	167	ASP	2.1
2	B	161	SER	2.1
2	H	188	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	3	GLN	2.1
2	B	96	HIS	2.1
2	H	191	THR	2.1
2	B	1	GLN	2.1
1	A	188	LYS	2.1
1	L	14	SER	2.1
2	H	193	THR	2.1
2	H	201	LYS	2.1
1	L	18	ARG	2.1
1	A	195	GLU	2.1
2	H	174	GLY	2.0
1	A	208	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CD	A	212	1/1	0.98	0.14	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.